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MULTIPLE COMPLEX DEMODULATION: A METHOD FOR RHYTHMIC ANALYSIS OF PHYSIOLOGICAL AND BIOLOGICAL DATA

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A methodology for analysis of periodic content in sequentially sampled data is described. Whereas previous chronobiological analyses have been limited to determining global parameters, multiple complex demodulation (MCD) provides local properties of amplitude and phase for each datum for each selected demodulating frequency. Real-time occurrences of maxima and minima, exact period calculation may be determined from remodulates. The entire analysis is computerized and graphic plots are output to enhance visualization of the utility of this information.

INTRODUCTION

Mathematical analyses of biological and physiological data suspected of inherent periodicities have been subject to various methods of time series analyses, depending on the nature of the information desired. Investigators concerned with phenomena attributed to circadian variations have depended greatly on the Cosinor method developed by Halberg et. al.[1] Those involved in the detailed examination of EEG traces have frequently made use of spectral analysis[2,3] in determining the relationships among records of simultaneous measurements from several electrode pairs. Included in this spectral analysis are the computations for correlograms, spectrograms, periodograms[4], and coherence. Harmonic[5,6,7,8,9] or Fourier analysis have been used by still others for extracting periodicities not immediately apparent.

Heart rate, EEG activity, eye movements, wrist and arm movements, body movements, hormonal and enzyme secretions, levels of biochemical constituents are stochastic processes. Their values at any future movement cannot be exactly calculated from previously known measurements. Instead, they are sampled over a sufficiently long interval to detect not only trends and abnormalities, but also the underlying rhythms, their magnitudes and instantaneous changes. Then, statements may be made as to the probabilities of such events occuring in the future.

Harmonic analysis or interchangably, Fourier analysis is applicable where it is assumed that the set of data consists of a series of sinusoidal components which may be collectively summed, i.e., that the series oscillate more or less harmonicly over time according to these components.

Spectrum analysis provides the possibility of any particular frequency to be in the data set, rather than setting forth exactly the actual presence of that frequency. Both the above processes result in general parameters pertinent to the entire ensemble.

For data which possess gradually changing amplitudes and phases (hence, implicit changes of frequencies), applying a technique that restricts the findings to only a single frequency and its concomitant amplitude and phase clearly limits the evaluation of information which can be used to enhance interpretation of the data.

In our laboratory we have utilized extensively the procedure of multiple complex demodulation (MCD) in analyzing sets of data as diverse as EKG, body temperature, activity movements, EOG, verbal communication in simulated battle environment, and hormonal secretion.

The complex demodulation technique has been set forth with great clarity by Bingham et. al.[10] and Bloomfield[11]; has been briefly illustrated by Walter[12], applied by Childers[13], Orr & Hoffman[14], and more recently by DePrins et. al.[15]. There is adequate theoretical basis for the use of this method in extracting from a sequential data series the local properties from each epoch in the time domain. The implication is that a non-stationary time series cannot accurately be described as having parameters which are constant over the entire set of data. The price to be paid for this flexibility according to Bloomfield[11] is less precision in the description of pure frequencies.

METHOD OF MCD ANALYSIS

In describing each of the steps involved in the multiple complex demodulation technique, the circadian period (24 hours) will be used in the example.

A. The Data Set

Measurements sampled sequentially in equal time increments preferebly for at least 2 cycles (48 hours) will comprise the data set depicted as:

$$X(t) = x_1, x_2, \ldots, x_N \qquad (1)$$

where each x element is an epoch value.

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The time increment may be one minute as in EKG data; 10 minutes as in actigraph (wrist and arm activity) records[16]; or integral hours as in body temperatures and hormonal secretions. The choice of sampling interval depends not only on the limitations of the measuring instrument, but also on the number of constituent frequencies desired for analysis.

Discrete equal sampling intervals introduce a problem known as "aliasing",[17] in which frequencies higher than the Nyquist frequency are enveloped by lower frequencies with which they coincide at crossover points. The highest frequency analyzable, in a record, then, is the Nyquist frequency. For a circadian cycle this limit is: $24/2\Delta t$, where 24 represents 1 cycle in hours, and Δt is the sampling interval in the same unit.

B. Detrending of Data Set

The data set is detrended by subtracting the mean value of the entire set from each epoch datum. This mean value is commonly referred to as the "zero frequency" and the result is a new data set which oscillates sinusoidal-like around a zero level. This set is now:

$$Y(t) = y_1, y_2, \ldots, y_N \qquad (2)$$

where

$$y_n = x_n - \frac{1}{N}\sum_{t=1}^{N} x_t \qquad n = 1, \ldots, N \qquad (3)$$

C. "Folding-Out" of Data Set

Necessarily, in the actual analysis, we must deal with a finite set of time series data. However, abrupt truncation of an infinite series on either end has consequences of "end effects" which result in distortion of their local properties. To minimize such effects, we have extended the length of our data set by "folding-out" the epoch values at both the beginning and termination of the data series. This is reasonable (Bloomfield[11]) in light of other alternatives which add zeroes to either side. This modification results in yet a new set of data values:

$$Z(fo) = y_m, y_{m-1}, \ldots, y_1, \underline{y_1}, y_2, \ldots, \underline{y_N}, y_N, y_{N-1}, \ldots, y_{m-\ell} \qquad (4)$$

where m is the number of folded-out data points and $\ell = m-1$. Note that the underlined, $\underline{y_1}$ $\underline{y_N}$ are the beginning and end respectively of the data set prior to the folding-out process.

The amount of data points folded-out varies according to the length of the data set. Our rule has been to use 20% of the total for a long data set ($\geq$ 100 values) and 5% for short segments.

The folded-out data set becomes the working set for all subsequent mathematical manipulations. The final output however retains only the parameters of the original epochs for statistical analysis and display.

D. Conversion to the Complex Domain

The first step in the actual process of decomposing the data set into its constituent frequencies involves the conversion of the values to the complex domain. This is necessary for the computation later of the proper amplitudes and phases. In the conversion, each epoch value is multiplied with separately (1) a cosine wave and (2) a sine wave containing the frequency to be elicited (the demodulated frequency) in their arguments. The result is the formation of 2 terms for each data epoch as follows:

$$Z(\mathrm{Re}) = Z_{t_i} \cdot \mathrm{Cos}\ \lambda t_i \qquad (5)$$

$$Z(\mathrm{Im}) = Z_{t_i} \cdot \mathrm{Sin}\ \lambda t_i \qquad (6)$$

where $\lambda = 2\pi f_j/\mathrm{S.R.}$, f = frequency selected for demodulation, $j = 1,2, \ldots, k$, $k \leq \mathrm{S.R.}/2$, and S.R. is defined as the sampling rate or number of sample epochs in the chosen period. For example, if the sampling interval is 15 minutes and the frequency of 2 cycles in the basic period (24 hours) is demodulated then $\lambda = 2\pi 2/96$.

Implicit in each datum is the collective value of all inherent frequencies contained in the data set. The multiplication by the sine and cosine terms preserves not only the original frequencies, but also generates sum and difference frequencies between the modulating frequency and all the original frequencies.

In the Fourier spectrum, this has the effect also of transposing the desired modulating frequency to the zero frequency position. This will be crucial as we will observe later in the filtering process.

Although we have fixed the period at 24 hours, the multiple complex demodulation allows the frequency within that period to vary and so we can demodulate each frequency of interest in a stepwise manner.

E. Filtering

The extraction of the desired frequency at the zero frequency position necessitates the exclusion of other components near to it in the energy spectrum. These may be noise or the difference frequencies described above which result in frequencies near the demodulating frequency.

For this purpose, an exponential filter is used and is passed sequentially through all the data points first in a forward pass, then a reverse pass and the whole process repeated. The forward pass causes a shift of one in the data set, which is corrected by the reverse pass thereby preserving the true phase values.

The low-pass characteristics of this filter allows the power at and near the zero frequency in the spectrum to pass through while excluding the rest of the spectrum. Inevitably, there will be some "leakage" of power through the filter, in particular from whatever residual power of frequencies located adjacent to the zero frequency.

For this reason, in analysis of data for circadian rhythmicity, the epoch values obtained from the circadian demodulation and properly transformed into remodulates (as will be discussed later) are subtracted from their corresponding values in the folded-out data set. The demodulations of all frequencies greater than one are then performed on this difference set.

The filter employed in our procedure consists of two parts:

$$F_1 = [(U)^2 + (V)^2]^{\frac{1}{2}} \quad (7)$$

$$F_2 = \exp(\alpha), \quad (8)$$

where

$$(U) = 1.0 - \exp(\alpha) \cdot \text{Cos}\ (GF \cdot T)$$

$$(V) = \exp(\alpha) \cdot \text{Sin}\ (GF \cdot T)$$

and

$$T = 2\pi/S.R.$$

$$\alpha = -T$$

GF = variable

and SR is defined as in (6). The gain factor, GF, may take values from 0.1 to 0.9 depending on the magnitude of the original data, i.e., the larger the data values, the smaller the gain factor required. It goes without saying that when different records are analyzed for direct comparisons, the same gain factor should be used in all cases.

In actual practice, the filter operation in a single pass involves summing a proportion of each epoch value with a proportion of the previous adjacent epoch value in the following way:

$$O_n\ (Re) = Z_n\ (Re) \cdot F_1 + Z_{n-1}(Re) \cdot F_2 \quad (9)$$

$$O_n\ (Im) = Z_n\ (Im) \cdot F_1 + Z_{n-1}\ (Im) \cdot F_2 \quad (10)$$

where n = m, m-1, ...1, ...N, N-1, ...,N-ℓ and m and ℓ have been defined in (4). The outputs from each filter pass are used as new inputs for the next pass going in the reverse direction.

F. Power, Amplitude, Phase, and Remodulate

The final outputs from the filtering operations may now be used for computing the parameters or local properties of each epoch. These are:

$$\text{Power:} \quad P_n = 2.0\ [O_n(Re)^2 + O_n\ (Im)^2] \quad (11)$$

$$\text{Amp:} \quad A_n = 2.0\ [O_n\ (Re)^2 + O_n\ (Im)^2]^{\frac{1}{2}} \quad (12)$$

$$\text{Phase:} \quad \Phi_n = \text{ARCTAN}\ [O_n\ (Im)/O_n\ (Re)] \quad (13)$$

$$\text{Remodulate:} \quad R_n = 2.0\ [O_n\ (Im) \cdot \text{Sin}\ (\lambda_f t) + O_n\ (Re) \cdot \text{Cos}\ (\lambda_f t)] \quad (14)$$

where the unit time increment, t = 0,1,..., N+2m, and f is the demodulated frequency.

The remodulate values, after truncation of the folded-out epochs at the beginning and termination of the data set, comprise a smoothed function of the desired demodulated frequency with the proper phases intact. Peak and trough amplitudes and their corresponding real time values may then be determined over the entire length of the data series for each frequency demodulated.

For a record consisting of several cycles, any shifts of trough and peak occurrences in real time may be detected on a daily basis. In addition, the length (in hours) of the actual circadian period may be calculated from peak to peak, trough to trough, or from zero cross over points from the remodulate. Changes in period lengths, thus also signal phase changes and may be confirmed from the phase plot. Also to be noted is the asymmetry between the positive portion of the cycle and the negative portion.

G. Selection Criteria for "True" Frequencies Inclusion

If biological and physiological rhythms are expressions of the energy state of the system, then consideration must be given as to which frequencies are "true" contributors and which are merely noise components. We have, in our laboratory, established rather strict criteria for the inclusion of any particular frequency as being a constituent of the total energy. Several steps are taken in this determination process and they are listed in the following order:

(1) The remodulate values of every frequency demodulated are scanned for their peak occurence values which are stored in arrays. The maximum value of all these peak values is selected as the basis for scaling into 20 grey levels, i.e., scale factor = 20./maximum value.

(2) The peaks of each remodulated frequency is multiplied with the scale factor and the products binned into the appropriate grey levels. Products less than 0.5 are binned into a zero level.

(3) The total population is determined from the sum of all the counts in the 21 bins.

(4) Beginning with the zero level, a cumulative tabulation is initiated with determination of the percent of total population at the end of each level's cumulation.

(5) When cumulation at the level containing 90% of the total population is attained, then that level is chosen as the cut-off value for determining inclusion of a frequency as a real component of the data set.

(6) Those frequencies possessing a peak value in their remodulates at or exceeding the grey level cut-off value are selected out as part of the biological system and are not considered random noise.

(7) The energy spectrum for biological systems may be considered partitioned as shown in Table I. On this basis the frequency bands will

be synthesized as the sum of remodulates of frequencies selected by the grey level process. Peaks and troughs and their respective positions in real time are also determined and recorded. Scanning down such lists allows immediate detection of the location (time) of unusual events.

(8) A graphic presentation of the grey level values above the cut-off point in a Time vs Frequency plot can illustrate with startling clarity, the wave-shaping properties of groups of frequencies.

STATISTICS

Since the multiple steps taken in the demodulation process resets the values of the output series with no direct or calculable relationship to the original data, it is not possible to make a direct comparison of these. But since in a time series, the important considerations are the changing nature of the values over the whole sample series and not the values per se, the statistical comparisons may be made on "normalized" data sets to capture any inter-relationships in synchrony over time. For this purpose, we have scaled each epoch value in each series with a scaling factor obtained by the ratio of 20: difference between maximum and minimum value in that series. Accordingly, the following statistical parameters are computed:

(1) Variance of the original data set.

(2) Variance of the circadian frequency and of each frequency band synthesized.

(3) Co-variance of the original data set with the circadian frequency and with each of the synthesized frequency bands.

(4) R^2 - Correlation of original data set with the circadian frequency and with each synthesized frequency band.

(5) R - Correlation coefficients of (4).

(6) RPER - a percent value, related to a goodness of fit measure. It is the ratio of the sum of the squares of differences to the sum of squares of maximum differences, where each maximum difference value is equal to 20. A value of 100% would indicate no fit.

REFINEMENTS - SPLINE FIT

Peak and trough selections in the above procedure will always be limited to the time of a sampled epoch whether or not the peak occurs there in reality or between sampling intervals. Since it is not known where the true peak occurs, we have applied a spline fit technique[18] to the remodulate values in an attempt to provide a better estimate of peak location. The result of the spline fit on a data series is a smoothed function which passes through all data points used in the fitting routine.

For example, if the sampled data consist of epochs taken at 15 minute intervals and it is desired to locate the actual peaking at better than the 15 minute interval, then a spline fit around the output peak (obtained in the procedure given above) is applied. The equal interval time axis is converted from unit incremental steps to the real time scale -- in this case to units of minutes. Two data points on each side of the peak and the peak point (five values in all) are subjected to the spline fit procedure to obtain the parameters for the smoothed function. These parameters are then used to determine the value of the function between time equivalent epochs on either side of the peak. Hence, we can now determine values of the function at one minute incrementing intervals instead of 15 minutes. The highest value computed from this function around the peak is taken to be the best estimate of the peaking and its corresponding time as the actual time of peaking.

Alternatively, for even coarser sampling intervals, i.e., every 4 hours, a spline fit may be made on the remodulate values and the values of the new function at fine resolutions of 15 minute interval increments may be calculated. The resulting values comprising a "stretched" remodulate series may then be scanned for their peaks and respective times in 15 min intervals instead of 4 hours.

The advantage of applying the spline fit technique is that we are not locked into describing peaks and troughs only at the sampling epoch time, but can obtain a finer resolution of peak time. The disadvantage is the slight distortion in amplitude of the peaks and troughs as a consequence of the requirement that the function must pass through each data point. This is a small price to be paid for the ability of exactly locating critical values in an oscillating system.

COMPUTER PROGRAMS

Computer programs are available for the methodology described, in which the input required are the sequential data set and the variables of sampling rate, epoch length, gain factor, starting time of the series, and number of frequencies (beginning with 1 cycle) to be demodulated. The output provides values of mean power for each cycle so that a "pseudo" power spectrum may be plotted. Additionally, all the maxima and minima of each remodulate, their real-time occurrences and amplitudes, and the period lengths are listed.

Plotting routines are used to display the results of the MCD technique. They illustrate the synthesis of the remodulates into characteristic bands of physiological significance and their summations are compared with the original data. The major modulator (circadian rhythm with period approximately 24 hr) is drawn superimposed over the entire data series and the corresponding phase is separately traced beneath it. Finally, rest and activity cycles are plotted on a daily basis to show any incipient phase shifting.

In the illustrations to follow, the sampling rate for a 24 hour period was used and the frequencies are cycles within this period.

Table I. Band Partition of Frequencies and Equivalent Periods

Bands	Frequency Cycles/Day	Period Hours	Hr/min/sec	Bands	Frequency Cycles/Day	Period Hours*	Hr/min/sec
Circadian	1	24.0	24/00/00	Supra-Ultradian	21	1.14	1/8/34
					22	1.09	1/5/27
Intermediate	2	12.0	12/00/00		23	1.04	1/2/36
	3	8.0	8/00/00		24	1.00	1/00/00
	4	6.0	6/00/00		25	0.96	0/57/36
	5	4.8	4/48/00		26	0.92	0/55/23
					27	0.89	0/53/20
Sub-Ultradian	6	4.0	4/00/00		28	0.86	0/51/26
	7	3.4	3/25/43		29	0.83	0/49/39
	8	3.0	3/00/00				
	9	2.7	2/40/00	Very High	30	0.80	0/48/00
	10	2.4	2/24/00		31	0.77	0/46/27
	11	2.2	2/10/54		32	0.75	0/45/00
					33	0.72	0/43/38
Ultradian	12	2.0	2/00/00		34	0.70	0/42/21
	13	1.8	1/50/46		35	0.68	0/41/08
	14	1.7	1/42/51		36	0.66	0/40/00
	15	1.6	1/36/00				
	16	1.5	1/30/00	*Rounded to tenths or hundredths			
	17	1.4	1/24/42				
	18	1.3	1/20/00				
	19	1.26	1/15/47				
	20	1.20	1/12/00				

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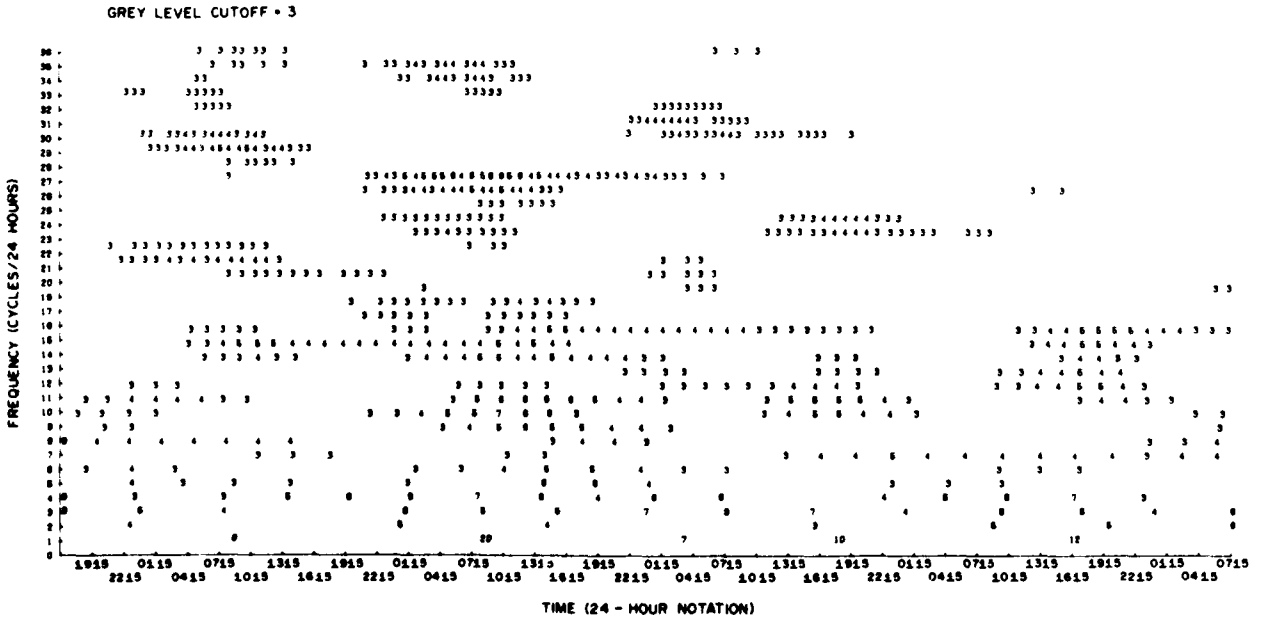

Fig. 1. Remodulate maxima of demodulated frequencies distributed as grey levels. The highest amplitude is indicated by 20. The lowest, 3, is the selection criterion level of significant components for inclusion in the 10% or less of the maxima population. The original data are 15 min epoch recordings of wrist and arm movements.

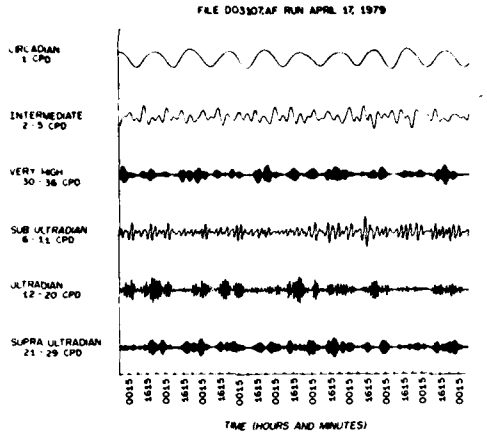

Fig. 2. Synthesis of remodulates of selected frequencies (cycles per day, CPD) into characteristic bands.

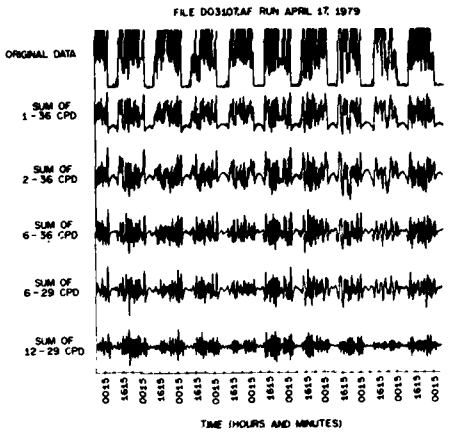

Fig. 3. Step by step summation of the characteristic bands shown in Fig. 2.

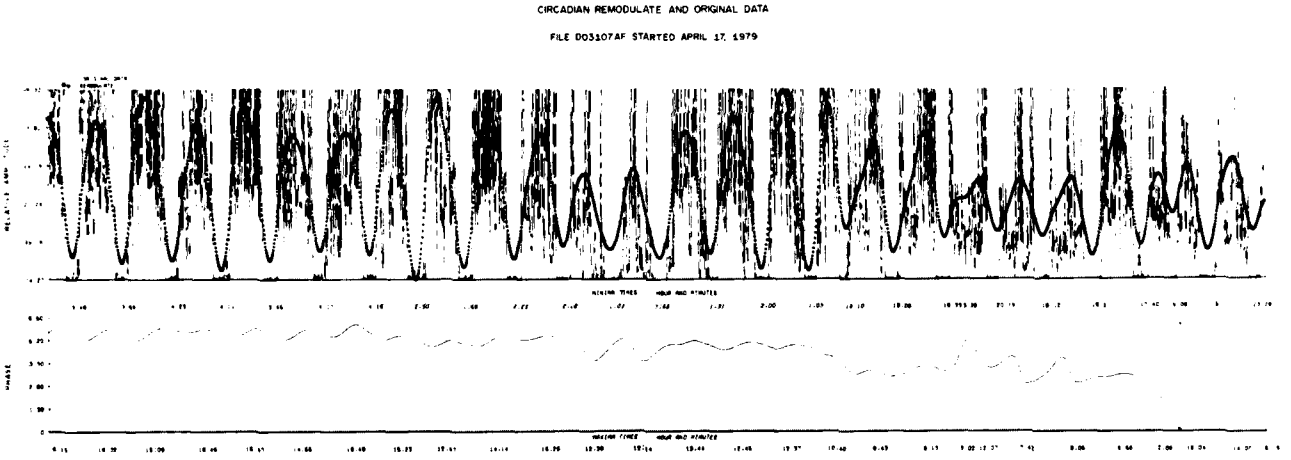

Fig. 4. Circadian remodulate superimposed over original data with corresponding phase plot and time of maxima and minima occurrences. From the wrist and arm movement records of a shift worker.

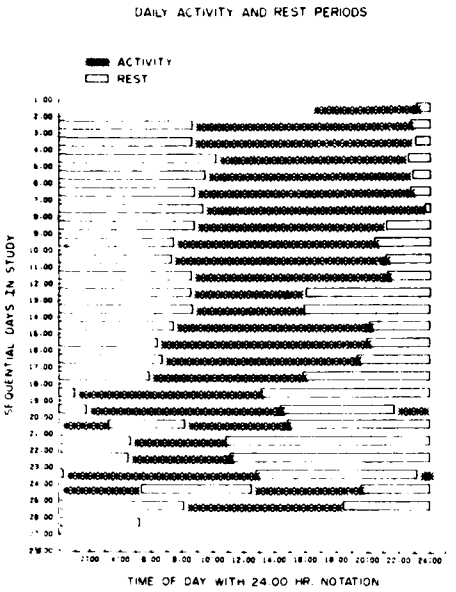

Fig. 5. Rest/activity cycles determined from zero cross-over points of circadian rhythm in Fig. 4. Note phase shift as the work shift is changed on day 18.

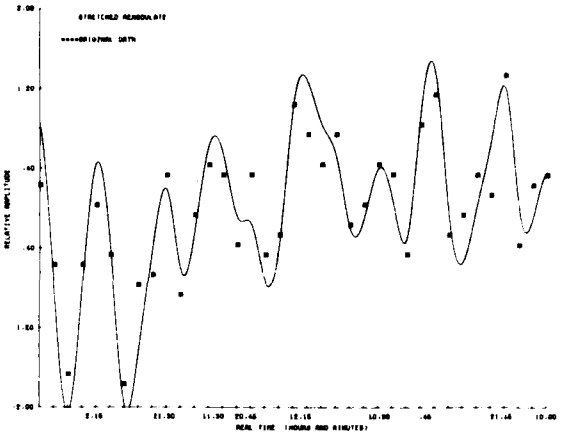

Fig. 6. Spline fit of circadian remodulate ("stretched remodulate") on 4-hour interval sampling of oral temperature. Maxima and minima may be determined to nearest 15 min.

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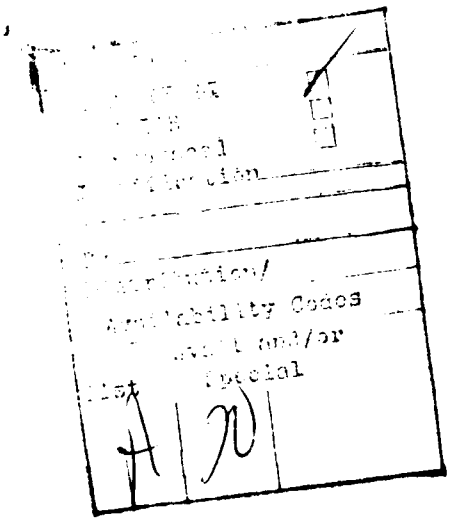


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